Invited Paper

Developing a Comprehensive Software Suite for Advanced Reactor Performance and Safety Analysis

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Abstract. This paper provides an introduction to the reactor analysis capabilities of the nuclear power reactor simulation tools that are being developed as part of the U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) Toolkit. The NEAMS Toolkit is an integrated suite of multi-physics simulation tools which leverage high-performance computing to reduce uncertainty in the prediction of performance and safety of advanced reactor and fuel designs. The Toolkit effort is comprised of two major components, the Fuels Product Line (FPL) that provides tools for fuel performance analysis and the Reactor Product Line (RPL) which provides tools for reactor performance and safety analysis. This paper provides an overview of the NEAMS RPL development effort.

1. Introduction

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) program [1] of the U.S. Department of Energy's Office of Nuclear Energy is developing a suite of advanced reactor and fuel simulation capabilities. The NEAMS Toolkit leverages current high-performance computing capacity in the U.S. to provide predictions of reactor and fuel performance with unprecedented fidelity. While the CASL (Consortium for Advanced Simulations of Light Water Reactors) project in the U.S. [2] and the NURISP (Nuclear Reactor Integrated Simulation Project) project in the E.U. [3] are focused on the deployment of advanced simulation tools for the current fleet of Light Water Reactors (LWR), the NEAMS program is focused on the development of advanced simulation tools to support the design and development of the advanced reactor types identified by the Generation IV program. The NEAMS Toolkit consists of two primary components, the NEAMS Fuels Product Line (FPL) and the NEAMS Reactor Product Line (RPL)

The objective of the NEAMS RPL is to enable the design of future nuclear power stations and reactor cores that implement enhanced safety and security features, produce power more cost effectively, and utilize natural resources more efficiently. In order to accomplish this, a significant shift in the

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approach to optimization of new core and plant designs is needed. The NEAMS RPL seeks to provide a toolset which:

(1)   Reduces margins due to predictive uncertainty by using mechanistic models and high fidelity simulation methods to increase accuracy and bridge gaps in experimental data and operating experience;
(2)   Enables designers to reduce design margins by providing tools which eliminate the need for geometric simplifications and material homogenization in simulations and limit dependence on engineering correlations which have a small range of applicability;
(3)   Introduces opportunities for a new level of global optimization of the reactor/fuel system, especially for new reactor or fuel concepts, through integrated (concurrent or hierarchal) predictions of reactor and fuel performance.

To accomplish these goals, the RPL must enable users to integrate simulations of physical phenomena on three levels. Multi-physics integration provides connectivity between different physics modules. Multi-scale integration provides connectivity between different scales of simulation within a single physics area, e.g., integration of multi-dimensional CFD simulations of a single power plant component with one dimensional lumped parameter simulations of the remainder of the plant. Multi-resolution integration (or hierarchal coupling) allows information from a predictive, mechanistic simulation to be used to inform a lower resolution models, e.g., using the results of a direct numerical simulation in place of a traditional correlation in a system level lumped parameter model.

2.   Requirements

NEAMS program requirements are defined through interactions with the leads and principal investigators of the U.S. DOE Nuclear Energy Reactor and Fuel Cycle Technology R&D programs, as well as potential academic and industrial users of the NEAMS RPL. Consideration is given to three major requirement categories. *Programmatic requirments* are those requirements resulting from the desire to align the NEAMS program with the efforts of the DOE-NE R&D programs. *Functional requirements* are those requirements imposed by the anticipated work flow of the NEAMS RPL's end users. *Applications requirements* are those requirements imposed by the target use cases to which the NEAMS RPL is expected to be applied. Of course, consideration is also give to funding requirements and limitations in developing the NEAMS Toolkit project plan.

2.1.   *Programmatic requirements*

The NEAMS project works to support all of the reactor and fuel cycle research and development programs of the U.S. DOE Office of Nuclear Energy. As a result, the scope of the NEAMS Reactor Product Line focuses on development of reactor technology neutral capabilities and includes support for a range of advanced reactor types, including

- Sodium-Cooled Fast Reactors,   (SFR)
- Prismatic Gas-Cooled Reactors,   (PMR)
- Pebble Bed Gas-Cooled Reactors,   (PBR)
- High-Temperature Fluoride-Salt-cooled Reactors,   (HFR)
- Lead-Cooled Fast Reactors,   (LFR)
- and Advanced Light Water Reactors.   (LWR)

NEAMS is focused on mid-term to long-term deployment options and focuses primarily on the development of capabilities which leverage advanced simulation methodologies and existing high performance computing infrastructure. The program currently works toward a 2018 release date for the initial user-ready Toolkit.

2.2. Functional Requirements

Key functional requirements have been identified through end-user meetings to focus and prioritize the scope of the development effort. These requirements characterize a spectrum of user expectations for the NEAMS RPL. There is no single characteristic user for NEAMS RPL, and the Toolkit must be able to support users who:

— Provide design and safety evaluations of current reactors for industry or research and development on advanced reactor designs for the U.S. DOE.

— Seek to complete both high-fidelity single-physics simulations and integrated multi-physics simulations of an entire plant.

— Have either broad experience and expertise in all of the physics included in a multi-physics reactor simulation or more limited expsoure in only one area.

— Utilize either conventional multi-core processor desktop workstations, commodity Linux clusters or leadership-scale petaflop computing facilities.

As a consequence, the NEAMS RPL must be able to meet a wide range of functional requirements. In response to this challenge, the NEAMS RPL has adopted a modular architecture that enables the user to customize the complexity of the model to fit their individual needs. A modern, modular architecture has been adopted to enable the flexibility needed to enable development of a reactor technology neutral toolset. However, there are common functional requirements which extend to all or large groups of potential users, including user interface requirements and user support requirements. Functional requirements for any software suite must be expected to evolve as the sophistication of high performance computing hardware — and its users — evolves. For this reason, regular stakeholders' meetings are held to assess the consistency of development priorities with end-user expectations. [4][5]

2.3. Applications Requirements

Applications requirements, which include the list of physical phenomena that must be represented in the toolset, are derived from the key use cases that the software suite is designed to support. As a consequence of the programmatic requirements that the development effort be reactor technology neutral, the development of a single broadly applicable use case is difficult. Therefore, four target use cases have been identified to drive the initial development efforts:

— Evaluation of passive safety features resulting from multi-physics, multi-scale reactor dynamics during Unprotected Loss of Flow (ULOF) transients in SFR cores

— Identification of thermal striping and stratification in outlet plena and other large volumes, especially in SFRs and PMRs

— Assessment of natural convection stability during startup of advanced reactor designs with limited pumping capacity, especially advanced Small Modular Reactors (SMR)

— Prediction of the impacts of core bypass flow on core performance and safety, especially in Very High Temperature Reactor (VHTR) cores using graphite pebble (PBR) or prismatic block (PMR) designs.

While no single use case covers the full range of reactor types included in the NEAMS RPL Toolkit's scope, the use cases identified do share some common features. All of the use cases are inherently multi-physics and require contributions from some combination of neutronics, thermal, fluid and structural mechanics models. They are also transient in nature, requiring that the physics modules resolve temporal changes in the fields that they simulate. Additionally, each of the use cases is tied to a complex geometry which has a strong influence on the relevant physical phenomena.

While consideration is given to all of the use cases in the development of the Toolkit, initial demonstration and validation efforts focus on analysis of the passive safety features of the SFR in a ULOF transient. In this transient analysis, the accurate prediction of feedback resulting from thermal expansion and mechanical distortion of the core structure is essential to accurate prediction of core power. [6] Therefore, the analysis requires a model which is inherently multi-physics and accounts for the complex geometry of the core and surrounding structure. Conventional methods accomplish this using models which are carefully calibrated to available operating experience and separate effects data. [7] The NEAMS Toolkit seeks to provide an assessment capability which can be more easily extended to new reactor concepts. In particular, the toolset should be applicable to evaluation of the passive safety characteristics of new SFR designs resulting from multi-physics thermal-structural-neutronics phenomena, such as those demonstrated in the Shutdown Heat Removal Tests (SHRT) at the Experimental Breeder Reactor II (EBR-II). [8]

The SFR passive safety transient focus was selected for a number of reasons. Current state-of-the-art codes cannot easily be used to address this problem for innovative reactor designs because the range of applicability of the empirical correlations used is limited. The problem is inherently multi-physics and requires integration of thermal, fluid, structural and neutronics phenomena. The problem is also inherently multi-dimensional and highly dependent on detailed representation of core geometry. The capabilities required are common to many reactor analyses and the tools needed are extensible to other reactor types. Perhaps most importantly, DOE owns significant, relevant experimental data for validation as a result of the development and operation of the EBR-II and the Fast Flux Test Facility (FFTF).

3. The NEAMS Reactor Product Line Software Design

The NEAMS RPL is comprised of two major products which can be applied independently or in concert – the lumped parameter RELAP-7 reactor system simulation code and the high-fidelity SHARP [9] reactor core simulation suite. In order to provide the flexibility needed to address the wide range of users and applications, a highly modular software architecture has been adopted. The basic components and associated connectivity functions which make up the NEAMS RPL, illustrated in Fig. 1, are described below.
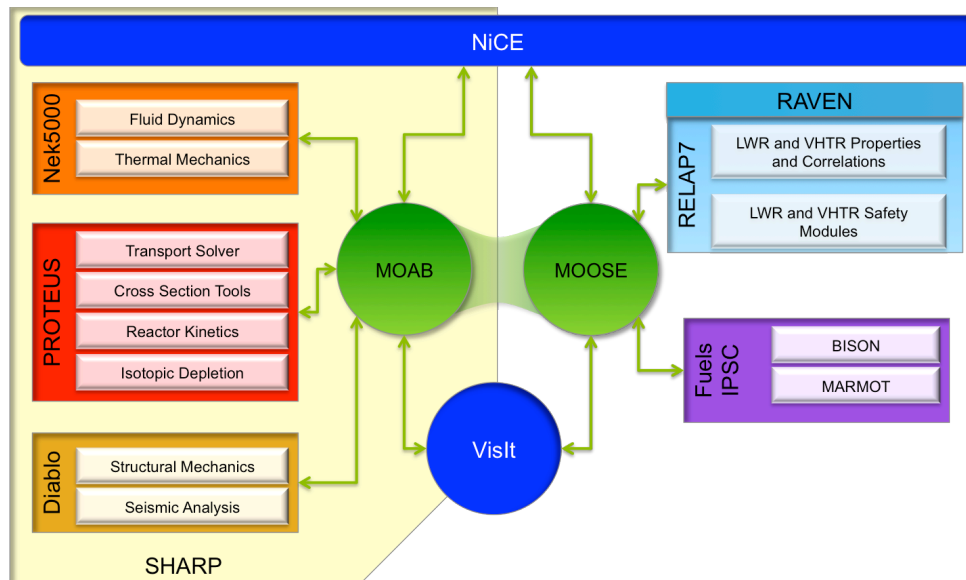

FIG. 1. Schematic View of NEAMS Reactor Product Line Components and Connectivity

3.1. Neutronics Modules

The NEAMS RPL neutronics tools, built using the PROTEUS package as a foundation, provide a complete analysis capability including three-dimensional transport, cross-section processing, reactor kinetics, and depletion. The NEAMS RPL neutronics tools include four major modules.

3.1.1. High Fidelity Cross-Section Module

The high-fidelity cross-section module, based on the code MC^2-3 from the PROTEUS suite, provides tools for generation of ultra-fine group cross-section libraries for fast reactor neutronics analyses.

3.1.2. Sub-Group Cross-Section Module

The sub-group module provides the tools needed to both generate cross-section libraries suitable for transport codes using the sub-group method and libraries that can be used to implement the sub-group method in transport codes, including the NEAMS-Neutronics high fidelity transport module. This method provides a lower computational cost alternative to the use of ultra-fine cross-section libraries generated by the high-fidelity cross-section module while retaining reasonable accuracy.

3.1.3. High Fidelity Transport Module

The high-fidelity transport module, based on the code UNIC [10] from the PROTEUS suite, provides tools for analysis of neutron transport phenomena within the reactor core. The module is, in essence multi-scale, because traditional homogenization approaches may be utilized to reduce computational cost – at the expense of accuracy. The module will eventually offer a variety of transport solver options, but initial development efforts will focus on a second-order, non-conformal, unstructured finite element discrete ordinates method. The module will be able to make use of both the high-fidelity and sub-group cross-section modules.

3.1.4. Near Term Kinetics Module

The near term kinetics module, based on the existing nodal diffusion method code DIF3D-K/VARIANT, provides functionality needed to complete near term transient reactor analyses while longer term development efforts are being executed. Development efforts related to this module are limited to integration of existing code with the NEAMS Integrated Framework, but may be expanded if required by the outcome of planned assessments of the high-fidelity transport module.

3.2. Thermal Fluid Modules

The NEAMS RPL thermal hydraulics tools provide a complete multi-scale thermal mechanics and fluid dynamics analysis capability. The one-dimensional lumped parameter capabilities of the thermal hydraulics tools are based on the system analysis code RELAP-7, and the three-dimensional mechanistic capabilities are based on the computational fluid dynamics (CFD) code Nek5000 [11][12][13][14]. The NEAMS-Thermal Hydraulics tools include three major modules.

3.2.1. RELAP-7 System Analysis Module

The RELAP-7 system analysis module, based on the code RELAP-7, provides one-dimensional lumped parameter system performance and safety analysis capability. The module provides a second-order finite element implementation of a 7-equation transport model. The module relies on conventional engineering correlations to account for multi-dimensional phenomena in the one-dimensional representation. Early development is focused on the capabilities needed for Light Water Reactor (LWR) safety analyses and will be completed in collaboration with the Light Water Reactor Sustainability (LWRS) program of the U.S. Department of Energy Office of Nuclear Energy. The NEAMS program is developing a limited set of SFR specific extensions to RELAP-7 to support analysis of the EBR-II passive safety transient demonstrations as a component of the NEAMS RPL.

3.2.2. High Fidelity CFD Module

The high fidelity CFD module provides predictive, mechanistic simulation of turbulent fluid dynamics and thermal mechanics using the highly scalable Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) capabilities of the spectral element method code Nek5000. In DNS, no engineering models are employed to describe the impacts of multi-dimensional turbulence and the full Navier-Stokes equation set is solved. In LES, the smallest turbulence length scales – those which are much smaller than the length scales of the computational mesh employed – are modeled rather than directly simulated. As a consequence, the computational cost of DNS and LES simulations is high, and the tools are best used as part of a multi-resolution hierarchy in which the serve to inform engineering models used by lower-fidelity methods and to aid in benchmarking of lower-fidelity simulations. The Nek5000 code is available as a stand-alone open source module.

3.2.3. Intermediate Fidelity CFD Module

The intermediate fidelity CFD module provides engineering scale simulations of multi-dimensional turbulent fluid dynamics and thermal mechanics using reduced-fidelity Reynolds Averaged Navier-Stokes (RANS) methods. In these methods, semi-empirical engineering models are used to describe all turbulence in the system. The primary RANS capability of the NEAMS-Thermal Hydraulics tools is implemented within the highly scalable spectral element solver of Nek5000. The module also provides limited connectivity to the commercial CFD code STAR-CCM+ [15], which is used by both nuclear energy research and development organizations and industry. This connectivity allows users to leverage their prior investments in complex CFD models of reactor cores and components.

3.3. NEAMS RPL Structral Mechanics Modules

The NEAMS RPL structural tools provide structural mechanics and material performance analysis. The structural mechanics module, based on the implicit finite element code Diablo, supports engineering scale analysis of structural performance of integrated structures such as fuel assemblies, reactor vessels, and containment building. The seismic analysis module extends the capabilities of the Structural Mechanics Module with a variety of soil modeling methods. A structural materials module, developed as an extension of the microstructure models for fuel components provided by the NEAMS Fuels Product Line, is planned for future versions, but is not expected to be part of the initial release.

3.4. NEAMS Integrated Framework Modules

The NEAMS Integrated Framework provides a suite of capabilities for integration of NEAMS Toolkit physics modules to enable simulation of multi-physics or multi-scale phenomena. The NEAMS Integrated Framework includes support for integration of physics modules using a unified operator (derived from MOOSE [16]) or a split operator (derived from MOAB [17]). The NEAMS Integrated Framework also includes tools to support management of mesh-based and geometry-based data and interpolation between mesh distributions or geometry representations used by different physics modules. The MOAB framework is available as a stand-alone open-source module.

3.5. NEAMS Meshing Modules

The NEAMS meshing modules provide capability for generation of computational meshes describing reactor geometries that can be used by the NEAMS physics tools. Current efforts focus on simplification of the process of generation for sodium cooled fast reactor core components using text file or user interface input.

3.6. NEAMS User-Interface Modules

The NEAMS Integrated Computing Environment (NICE) module [18] provides the user interface for problem definition, the user interface for compute job control, and the user interface for data analysis and visualization. The environment also provides access to a suite of utilities to support data analysis,

parametric studies, workflow management, generation of model documentation, and access to code documentation. The NICE interface module is available as a stand-alone open source module.

4. Major Innovations and Accomplishments

The NEAMS project has adopted a modern code development strategy which relies upon highly modular componentwise development to provide extreme flexibility in the use and application of the code suite. The NEAMS Toolkit suite applies the principles of object-oriented programming, and leverages many existing solution and support libraries such as PETSc [19], Trillinos [20], LibMesh [21], and MOAB [17]. The NEAMS project also leverages the MOOSE [16] software development platform, which itself uses PETSc, Trillions, and LibMesh. With many internal and external dependencies, more traditional approaches to softwared verification, which often rely on line by line reviews completed by secondary reviewers at the end of the development cycle, are difficult to implement and often less reliable than desired. The project has adopted software quality assurance (SQA) practices that build upon a foundation of rigourous version control and tracking, automated verification and automated documentation.

One common thread in the difficult challenge problems that have been identified is the importance of geometry, or small changes in geometry, to the prediction of multi-physics behaviors. To address this challenge, the toolset enables generation of computational models which represent the geometry of the system with unprecedented fidelity. Unstructured computational mesh approaches are becoming increasingly common in engineering analysis software packages to enable more realistic representations of component geometry. The NEAMS RPL leverages these approaches and includes a unique neutron transport solution capability [22][23] which can both utilze these fully-unstructured computational meshes for more accurate representation of core geometry and make use of high resolution ultra-fine group nuclear cross-section data where it is available. This important feature enables the toolset to provide more accurate predictions of local reaction rates in fuel and structural material regions, and more accurately assess reactivity coefficients – especially those related to core component distortions. Initial demonstrations have focused on the application of the toolset to well-described benchmark problems with complex geometries, such as the ZPR-6/7 experiments [24] shown in Fig.2, and to core of the Advanced Test Reactor (ATR)[25].

The NEAMS Toolkit also enables the application of high-fidelity computational fluid dynamics and structural mechanics analysis to advanced reactor preformance and safety assessments. These simulation tools provide insight into to multi-dimensional phenomena that cannot be easily evaluated using conventional correlation based methods. The high-fidelity capabilities of the Toolkit enable accurate assessment of localized temperature, flow and material stress effects resulting from component contact, flow stagnation, flow stratification and structural deformation. Evaluation of relevant phenomena in reactor components using these tools requires access to significant
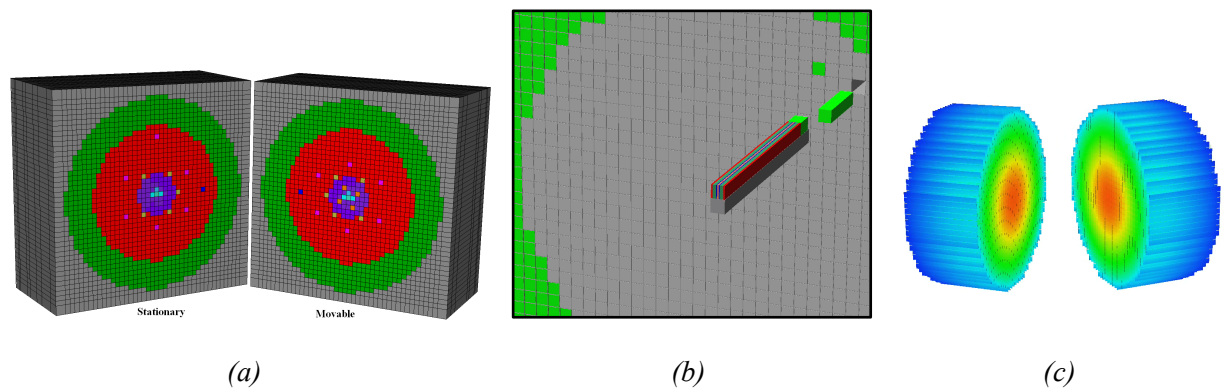

(a)	*(b)*	*(c)*

FIG. 2. (a) Geometry of the ZPR-6/7 loading 106 SFR critical experiment, (b) detailed geometry of heterogenous fuel drawer geometry from simulation, and (c) predicted flux in thin fuel plate at center of each drawer.
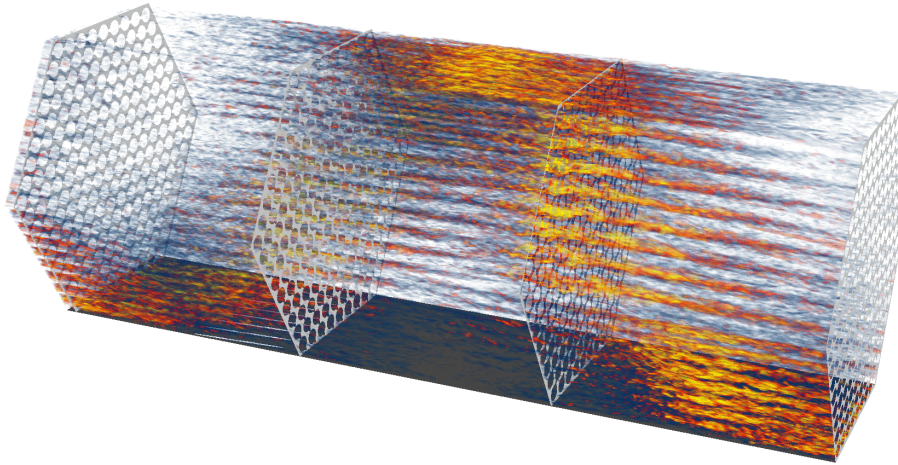
FIG. 3. Predicted evolution of turbulence in a Nek5000 spectral-filtered LES simulation of a 217-pin wire-wrapped fuel assembly using n=1.01 billion grid points. [33]

computational resources with hundreds of thousands of CPU cores. Therefore, they have been adopted as part of the NEAMS multi-scale, multi-resolution strategy and are expected to provide benchmarking or calibration data for lower fidelity methods which are part of the NEAMS RPL. Initial demonstrations of these capabilities have focused on separate effects validation exercises in which thermal stratification or striping is observed [26][27], and a thorough assessment of the evolution of flow fields in wire-wrapped SFR fuel assemblies of various configurations[28][29][30][31][32], as shown in Fig. 3.

Since the physics analysis toolset relies on unstructured computational mesh descriptions, generation of those meshes and management of data associated with those meshes is critical to the success of the package. A reactor geometry mesh generation toolset, called MeshKit, has been developed as part of the NEAMS RPL. The MeshKit tools reduce mesh development time for full core geometries, without spacer components, from days to minutes. [34] The tools have been demonstrated for SFR, PMR, LWR and complex test reactor cores such as the Advanced Test Reactor.

For the NEAMS RPL, the one of the most signficant challenges lies in managing the large mesh-based data sets generated by each of the high-fidelity physics modules. The data stored on the mesh must be available to the single physics application from whence it came and also be accessible to the other physics modules that are integrated to complete a multi-physics simulation. Perhaps the most important innovation of the NEAMS RPL is a powerful suite of mesh-based data management and code integration tools which enable the integrated multi-physics modules to move beyond simply share cell-centered data from the previous iteration, as is typically done in recent coupled code demonstrations. The code integration framework provided by the MOAB toolset enables the data exchange functions to take advantage of higher order information in the solution and MOAB's awareness of the underlying geometry when transfering data between modules using different computational meshes. The goal of this development effort is to significantly reduce the error associated with translation of data between meshes. An initial demonsration of MOAB-enabled data exchange among the primary physics modules of the NEAMS RPL toolset was recently completed for a simplified SFR fuel assembly geometry, as shown in Fig. 4, and more protypic demonstrations of this capability are expected during the next year.

5. Summary and Conclusions

The NEAMS RPL is an integrated suite of tools which enables high-fidelity multi-physics, multi-scale simulations for the assement of performance and safety characteristics of advanced nuclear reactor concepts. The initial release of the fully featured toolset to the user community, planned for 2018, will support analysis of a variety advanced reactor types and conditions. However, the initial validation efforts center on a single focus problem – the ULOF transient in an SFR. Initial demonstrations of

capability for this challenge problem have already been completed, and more protypic demonstrations are in progress. Some components, including the Nek5000 CFD module, the MOAB framework module and the NICE user interface module, have already been released as stand-alone open-source modules for use by the community-at-large.
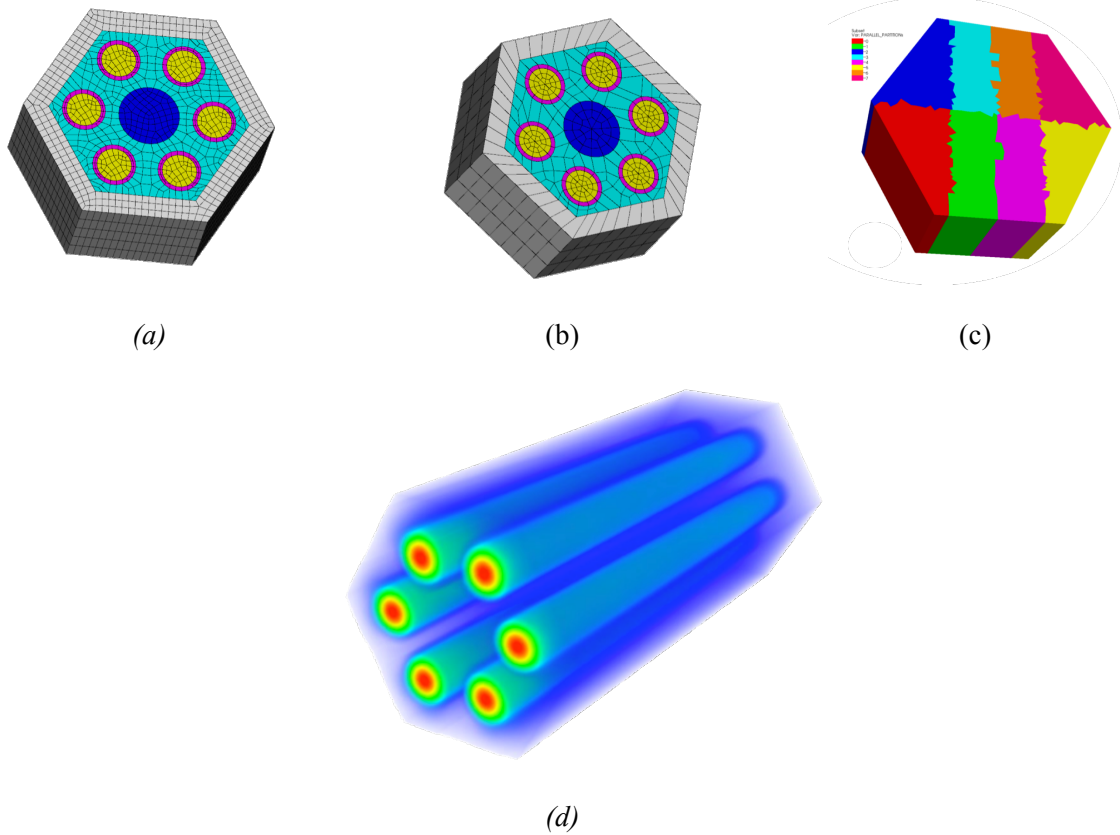

(a)   *(b)*   (c)

(d)

FIG. 4. (a) CFD mesh, (b) neutronics mesh, (c) decomposition, and (d) thermal field solution for simplified SFR fuel assembly multi-physics simulation using the NEAMS RPL.

Acknowledgements

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